# Amino Acid Adsorption on Chiral Mineral Surfaces

Robert M. Hazen
*Geophysical Laboratory*
*Carnegie Institution of Washington*
*5251 Broad Branch Rd. NW Washington DC 20015*
*USA*
r.hazen@gl.ciw.edu

Aravind R. Asthagiri
*Geophysical Laboratory*
*Carnegie Institution of Washington*
*5251 Broad Branch Rd. NW Washington DC 20015*
*USA*

Robert T. Downs
*Geophysical Laboratory*
*Carnegie Institution of Washington*
*5251 Broad Branch Rd. NW Washington DC 20015*
*USA*

The source of life's homochirality is one of the central questions of origin of life research. Naturally occurring chiral faces of minerals may have been a source of symmetry breaking in the very early stages of life. Experimental work by Hazen and co-workers has demonstrated that chiral mineral surfaces can differentiate between enantiomers of amino acids, but the details of the atomic level interactions of the amino acid/surface interface are not known. As a first step to rectify this lack of information we have modeled the adsorption of alanine and asparatic acid on the chiral calcite(214) surface using Density Functional Theory (DFT), an accurate first-principles method. We have mapped out the potential energy surface for both L and D-alanine on calcite(214). We find that alanine shows negligible enantiospecific adsorption (*i.e*. L and D enantiomer have similar adsorption energy) due to the lack of three strong points of interactions with the calcite surface. Asparatic acid has two carboxyl groups and there is a fortuitous match between the O-O distances on asparatic acid and the Ca-Ca atoms. The additional Ca-O interaction leads to a more constrained adsorption geometry and we find D-asparatic acid is favored by 8 Kcal/mol. Our results match the observations from the experimental work of Hazen *et al*. on the same calcite(214) surface and show the promise of using modeling as a complement to experiment to gain a better understanding of these systems. We will discuss ongoing efforts to extend the modeling work to other amino acid/mineral systems and compare to parallel experimental work from our lab.